MATERIAL SAFETY DATA SHEET

1. SUBSTANCE AND SOURCE IDENTIFICATION

National Institute of Standards and Technology
Standard Reference Materials Program
100 Bureau Drive, Stop 2320
Gaithersburg, Maryland 20899-2320

SRM Number: 39j
MSDS Number: 39j
SRM Name: Benzoic Acid
Calorimetric Standard

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Description: Standard Reference Material 39j is intended for use in the calibration and standardization of adiabatic, isoperibol, and aneroid bomb calorimeters. It was refined by fractional freezing to give a material of high homogeneity and purity and conforms to the American Chemical Society specification for reagent-grade benzoic acid. Mass spectrometric and coulometric measurements indicate a purity of 0.999 996 mol/mol SRM 39j is supplied in a unit consisting of 30 g of crystalline material.

Substance: Benzoic Acid

Other Designations: **Benzoic Acid** (benzenecarboxylic acid; benzenemethanoic acid; benzeneformic acid; benzoate; carboxybenzene; dracyclic acid; phenyl carboxylic acid; phenylformic acid;. phenylcarboxylic acid)

2. COMPOSITION AND INFORMATION ON HAZARDOUS INGREDIENTS

Component	CAS Number	EC Number (EINECS)	SRM Concentration (mass %)
Benzoic Acid	65-85-0	200-618-21	100

EC class: Xn **EC Risk (R No.):** 22,36/37/38 **EC Safety (S No.):** 2,13,24/25/26,36,46

See Section 15, "Regulatory Information".

3. HAZARD IDENTIFICATION

NFPA Ratings (Scale 0-4): Health= 2 Fire = 1 Reactivity = 0
Major Health Hazards: Respiratory tract irritation. Skin irritation. Eye irritation.
Physical Hazards: Dust/air mixtures may ignite or explode.
Potential Health Effects

Inhalation: Irritation.
Skin absorption: Irritation.
Eye contact: Irritation (possibly severe).
Ingestion: Irritation. Nausea. Vomiting. Stomach pain.
Long term exposure: Irritation. Nausea. Vomiting, tremors. Blood disorders. Convulsions.

Listed as a Carcinogen/Potential Carcinogen:

	Yes	No
In the National Toxicology Program (NTP) Report on Carcinogens		X
In the International Agency for Research on Cancer (IARC) Monographs		X
By the Occupational Safety and Health Administration (OSHA)		X

4. First Aid Measures

Inhalation: If adverse effects occur, remove to uncontaminated area. If not breathing, give artificial respiration by qualified personnel. Get immediate medical attention.

Skin Contact: Rinse affected area with soap and water for at least 15 minutes while removing contaminated clothing and shoes. Obtain medical assistance if necessary. Thoroughly clean and dry contaminated clothing and shoes before reuse.

Eye Contact: Immediately flush eyes, including under the eyelids, with copious amounts of water for at least 15 minutes. Obtain medical assistance immediately.

Ingestion: If a large amount is swallowed, get medical attention.

5. Fire Fighting Measures

Fire and Explosion Hazards: Slight fire hazard. Dust/air mixtures may ignite or explode.

Extinguishing Media: Regular dry chemical. Carbon dioxide. Water. Regular foam.

Large Fires: Use regular foam or flood with **FINE** water spray. **DO NOT** scatter spilled material with high-pressure water streams.

Fire Procedures: Do not touch spilled material. Move container from fire area if it can be done without risk. Dike for later disposal.

Flash Point (°C): 121 (250 °F) **Method:** CC **Autoignition (°C):** 571 (1060 °F)

Flammability Limits in Air (Volume %): **UPPER:** 1232 g/m^3 (35 g/ft^3)
LOWER: > 104 g/m^3 (>3 g/ft^3)

6. Accidental Release Measures

Occupational Release: Keep out of water supplies and sewers. Keep unnecessary people away, isolate hazard area and deny entry. The reportable quantity (RQ) for benzoic acid under Title III of SARA Section 304 is greater than the unit quantity provided for SRM 39j. Notify Local Emergency Personnel and State Emergency Response Commission for release greater than or equal to RQ (U.S. SARA Section 304). If release occurs in the U.S. and is reportable under CERCLA Section 103, notify the National Response Center at (800) 424 8802 (USA) or (202) 426 2675 (USA).

Environmental Precautions: See section 13, "Disposal Considerations".

Clean-up Methods: Collect spilled material in appropriate container for proper disposal.

7. Handling and Storage

Storage: Store and handle in accordance with all current regulations and standards. Keep container tightly closed. Store in a cool, dry place. Store in a well-ventilated area. Protect from physical damage. Store with acids. Keep separated from incompatible substances.

Precautions for Safe Handling: Use methods to minimize dust.

8. Exposure Controls and Personal Protection

Hazardous Component	Exposure Limits
Benzoic Acid	No occupational limits established.

Ventilation: Ensure compliance with applicable exposure limits. Ventilation equipment should be explosion-resistant if explosive concentrations of material are present.

Respiratory protection: Under conditions of frequent use or heavy exposure, and engineering controls are not feasible, respirator protection is required. Refer to the NIOSH Guide under 42CFR84 for selection and use.

Eye Protection: Wear safety goggles. **DO NOT** wear contact lenses in the laboratory. Provide emergency eye wash fountain and quick drench shower in the immediate work area. An eye wash station should be readily available near the handling and use areas.

Personal Protection: Wear chemically resistant gloves and appropriate clothing to prevent skin exposure.

9. PHYSICAL AND CHEMICAL PROPERTIES

Benzoic Acid	
Appearance and Odor: Colorless to white crystals. Faint, pleasant odor.	**Density:** 1.3 g/cm^3
Molecular Formula: C_6H_5 COOH	**Volatility (at 21 ºC):** 0 %
Molecular Weight: 122.12	**Water Solubility (at 20 ºC):** 2.9 %
Boiling Point (°C): 250	**pH (at 25 ºC):** 2.8 (saturated solution)
Melting Point (°C): 122	**Solvent Solubility:** Soluble in acetone, alcohol, benzene, carbon disulfide, carbon tetrachloride, chloroform, ethanol, ether, fixed and volatile oils, oil of turpentine. Slightly soluble in petroleum ether, hexane.
Vapor Pressure (at 96 ºC): 1 mmHg	
Vapor Density (air = 1): 4.2 – 4.21	

10. STABILITY AND REACTIVITY

Stability: **X** **Stable** ____ **Unstable**

Stable at normal temperature and pressure.

Conditions to Avoid: Avoid heat, flames, sparks and other sources of ignition. Avoid contact with incompatible materials.

Incompatibility (Materials to Avoid): Bases. Metals. Oxidizing materials.
Bases: Exothermic reaction.
Metals (Solutions): Reacts to form hydrogen gas.
Oxidizers (Strong): Vigorous exothermic reaction.

Hazardous Decomposition or Byproducts: Thermal decomposition produces oxides of carbon, aromatic compounds, phenols.

Hazardous Polymerization: ____ **Will Occur** **X** **Will Not Occur**

11. TOXICOLOGICAL INFORMATION

Route of Entry: **X** **Inhalation** **X** **Skin** **X** **Ingestion**

Toxicological Data
Human, Skin TD_{Lo}: 6 mg/kg
Human, Ingestion LD_{Lo}: 500 mg/kg
Human, Skin: Moderate irritation 22 mg/3 d
Rat, Oral LD_{50}: 1700 mg/kg
Rabbit, eyes: Severe irritation 0.25%/ 1 h

Mutagenic Data
Escherichia coli, Mutation in Microorganisms: 10 mmol/L (-S9)
Human Lymphocyte, DNA Inhibition: 5 mmol/L

Medical Conditions Generally Aggravated by Exposure: Not applicable.

12. ECOLOGICAL INFORMATION

Ecotoxicity Data

Fish LC_{50}: 96 h 180 mg/L
Daphnia EC_{100}: 24 h 1000 mg/L
Algae EC_{50}: 12-14 wk >10 mg/L

Environmental Summary: Relatively non-persistent in the environment. Not expected to leach through the soil or the sediment. Accumulates very little in the bodies of living organisms. Slightly volatile from water.

13. DISPOSAL CONSIDERATIONS

Waste Disposal: Dispose in accordance with federal, state and local regulations. Keep out of water supplies and sewers.

14. TRANSPORTATION INFORMATION

U.S. DOT Registry: Not regulated by DOT. Aromatic, carboxylic acids. Class Hazard 0.

Land, Air, Meritime Transport: No classification assigned.

15. REGULATORY INFORMATION

U.S. REGULATIONS

CERCLA Sections 102a/103 Hazardous Substances (40CFR302.4): Benzoic acid 2270 kg (5000 lbs).
SARA Title III Sections 302, 304, 313: Not regulated.
SARA Title III Sections 311/312 Hazrdous Catergories (40 CFR 370.21):
ACUTE: Yes.
CHRONIC: No.
FIRE: No.
REACTIVE: No.
SUDDEN RELEASE: No.
OSHA Process Safety. California Proposition 65: Not regulated.

CANADIAN REGULATIONS

WHMIS: Not determined.

EUROPEAN REGULATIONS

EC CLASSIFICATION

Xn Harmful.

EC RISK AND SAFETY PHRASES

R22 Harmful if swallowed.
R36 Irritating to eyes.
R37 Irritating to respiratory system.
R38 Irritating, to skin.
S2 Keep out of reach of children
S13 Keep away from food, drink and animal feedingstuffs.
S24 Avoid contact with skin.
S25 Avoid contact with eyes.
S26 In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
S36 Wear suitable protective clothing.
S46 If swallowed, seek medical advice immediately and show this container or label.

16. OTHER INFORMATION

Sources: MDL Information Systems, Inc., MSDS *Benzoic Acid*, 19 March 2003.

Disclaimer: Physical and chemical data contained in this MSDS are provided only for use as a guide in assessing the hazardous nature of the material. The MSDS was prepared carefully, using current references; however, NIST does not certify the data in the MSDS. The certified values for this material are given in the NIST Certificate of Analysis.